

# Andreev Bound States at the Interface of Antiferromagnets and d-wave Superconductors

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We set up a simple transfer matrix formalism to study the existence of bound states at interfaces and in junctions between antiferromagnets and d-wave superconductors. The well-studied zero energy mode at the  $\{110\}$  interface between an insulator and a  $d_{x^2-y^2}$  wave superconductor is spin split when the insulator is an antiferromagnet. This has as a consequence that any competing interface induced superconducting order parameter that breaks the time reversal symmetry needs to exceed a critical value before a charge current is induced along the interface.

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The discovery of the symmetry of the superconducting order parameter has been one of the most successful studies of the High- $T_c$  materials. Angular resolved photoemission spectroscopy has revealed the nodes in the gap function and tunneling experiments have proven the sign change between adjacent lobes of the  $d_{x^2-y^2}$  wave gap<sup>1-3</sup>. It was first shown by Hu<sup>4</sup> that this sign change can lead to zero energy Andreev bound states (ZEBS) at the surface of an insulator and a d-wave superconductor. These Andreev bound states were later identified with the zero bias conductance peaks observed in tunneling experiments. The experiments by Covington *et.al.*<sup>5</sup> indicated, however, that the surface states were spontaneously split by a minigap. Several ideas were proposed for this effect<sup>6</sup>; one of which included the induction of a time reversal symmetry breaking  $is$  component of the order parameter near the interface<sup>7</sup>. The resulting gap  $d + is$  lowers the condensation energy by lifting the directional degeneracy of the ZEBS<sup>8</sup>. Later Honerkamp *et.al.*<sup>9</sup> used a tight-binding model with onsite repulsion and spin dependent nearest neighbor interaction to self-consistently study the competition between additional induced orders near the surface of an insulator and a  $d_{x^2-y^2}$  wave superconductor.

Motivation for studying close domains of antiferromagnetism and superconductivity arises from the existence of striped domains in the cuprate materials. This was further emphasized by recent elastic neutron scattering experiments showing that static antiferromagnetic order is induced in a superstructure around the vortices in the mixed state of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ <sup>10</sup> and  $\text{La}_2\text{CuO}_{4+\delta}$ <sup>11</sup>. These experiments are consistent with a static environment of alternating antiferromagnetic and d-wave superconducting stripes around the vortex cores. Thus the electronic states in such an environment is an important question.

Inspired by these experiments we set up a simple transfer matrix method to identify bound states on interfaces and junctions between antiferromagnets and d-wave superconductors. In particular we discuss a single interface separating antiferromagnetic and d-wave superconduct-

ing half-planes (AF/dSC), and point out a few differences from the conventional non-magnetic insulator-d-wave superconductor interface (I/dSC). Note that the antiferromagnetism forces us to study a lattice model which is contrary to the usual discussion of Andreev interference in terms of semi-classical continuum models.

A simple lattice model that includes both d-wave superconductivity and antiferromagnetism is given by the following Hamiltonian

$$H = -t \sum_{\langle n,m \rangle \sigma} c_{n\sigma}^\dagger c_{m\sigma} + H.c. - \mu \sum_{n\sigma} c_{n\sigma}^\dagger c_{n\sigma} \quad (1)$$

$$+ \sum_{\langle n,m \rangle} \Delta_{n,m} c_{n\uparrow}^\dagger c_{m\downarrow}^\dagger + H.c. \quad (2)$$

$$+ \sum_n M_n \left( c_{n\uparrow}^\dagger c_{n\uparrow} - c_{n\downarrow}^\dagger c_{n\downarrow} \right) \quad (3)$$

where  $\langle n,m \rangle$  denotes nearest neighbors.  $M_n$  and  $\Delta_{n,m}$  are the spatially dependent magnetic and superconducting order parameters. This Hamiltonian is quadratic and can be diagonalized by a Bogoliubov-de Gennes (BdG) transformation

$$\gamma_\sigma^\dagger = \sum_n u_\sigma(n) c_{n\sigma}^\dagger + \sigma v_\sigma(n) c_{n-\sigma}. \quad (4)$$

with  $\sigma$  equal to +1 (-1) for spin up (down). We use the notational convention that the spin indices on  $u_\sigma$  and  $v_\sigma$  follow that on the Bogoliubov operators  $\gamma_\sigma^\dagger$ .

In the case of a  $d_{x^2-y^2}$ -wave superconductor there are two qualitatively different orientations of the interface; the  $\{100\}$  and  $\{110\}$  directions corresponding to a vertical and diagonal stripe respectively. Both cases are studied below with the  $x$ -axis ( $y$ -axis) chosen perpendicular (parallel) to the interface which is placed at  $x = 0$ . The lattice constant is set to unity. Assuming translational invariance along the  $y$ -direction the AF/dSC interface reduces to a one dimensional problem. For the  $\{100\}$  interface the resulting Bogoliubov-de Gennes equations have the form

$$\epsilon_\sigma u_{q\sigma}(x) = -t(u_{q\sigma}(x+1) + u_{q\sigma}(x-1) + 2\cos(q)u_{q\sigma}(x)) - \mu u_{q\sigma}(x) + \sigma M_x u_{q+Q\sigma}(x) \quad (5)$$

$$\begin{aligned} & + (\Delta_{x+1,x}^d) v_{q\sigma}(x+1) + (\Delta_{x-1,x}^d) v_{q\sigma}(x-1) + 2\cos(q)(-\Delta_x^d) v_{q\sigma}(x) \\ \epsilon_\sigma v_{q\sigma}(x) & = t(v_{q\sigma}(x+1) + v_{q\sigma}(x-1) + 2\cos(q)v_{q\sigma}(x)) + \mu v_{q\sigma}(x) + \sigma M_x v_{q+Q\sigma}(x) \\ & + (\Delta_{x+1,x}^{*d}) u_{q\sigma}(x+1) + (\Delta_{x-1,x}^{*d}) u_{q\sigma}(x-1) + 2\cos(q)(-\Delta_x^{*d}) u_{q\sigma}(x) \end{aligned} \quad (6)$$

after fourier transforming along the  $y$  direction. The corresponding equations for the fourier components  $u_{q+Q\sigma}$  and  $v_{q+Q\sigma}$  are obtained by simply performing the substitution  $q \rightarrow q+Q$ . These BdG equations are diagonal in the spin index with the only difference between spin up and down being the sign of the magnetic term.

A simple way to study bound states at the interface is in terms of the transfer matrix method<sup>12</sup>. Thus we introduce a  $(q, \epsilon)$ -dependent matrix  $T(x+1, x)$  defined by

$$\Psi(x+1) = T(x+1, x) \Psi(x). \quad (7)$$

which transfers the spinor  $\Psi$  from site  $x$  to site  $x+1$ . For a model with nearest neighbor coupling  $\Psi$  takes the explicit form  $\Psi(x) = (\psi(x), \psi(x-1))$  where

$$\psi(x) = (u_{q\sigma}(x), v_{q\sigma}(x), u_{q+Q\sigma}(x), v_{q+Q\sigma}(x)). \quad (8)$$

The associated  $8 \times 8$  transfer matrix has the general form

$$T(x+1, x) = \begin{pmatrix} A & B \\ 1 & 0 \end{pmatrix} \quad (9)$$

where  $A$  ( $B$ ) denotes the  $4 \times 4$  coefficient-matrix connecting  $\psi(x+1)$  and  $\psi(x)$  ( $\psi(x-1)$ ) determined from the BdG equations (5-6). In the simplest case of a sharp interface we have the following spatial dependence of  $M_x$  and  $\Delta_x$

$$M_x = M(-1)^x \quad \text{for } x \leq 0 \quad (10)$$

$$\Delta_x = \Delta_d \quad \text{for } x > 0 \quad (11)$$

Thus there are effectively three different transfer matrices; one in the bulk magnetic region  $T_M$ , one in the bulk superconducting region  $T_{SC}$  and one associated with transfer through the interface  $T_I$ . By diagonalizing  $T_M$  and  $T_{SC}$  there exists decaying, growing or propagating eigenstates depending on whether the eigenvalues are less, larger or equal to one, respectively. Here, decaying and growing are referred to propagation along the  $x$ -axis for increasing  $x$ . If  $PET_M$  denotes the matrix obtained after propagating the eigenvectors of the bulk magnetic transfer matrix through the interface we introduce a matrix  $\alpha$  given by

$$PET_M = ET_{SC} \alpha \quad (12)$$

where  $ET_{SC}$  is the matrix containing the eigenvectors of the bulk superconducting region as column vectors. The

dot indicates matrix multiplication. Now, let  $S_g^m$  and  $S_g^{sc}$  denote the subspace of growing eigenstates of  $PET_M$  and  $ET_{SC}$  respectively, and consider the following linear combination of the growing states of  $PET_M$

$$\begin{aligned} \sum_{i \in S_g^m} \beta_i |PET_M i\rangle & = \sum_{i \in S_g^m} \sum_{j \in S_g^{sc}} \beta_i \alpha_{ji} |ET_{SC} j\rangle \quad (13) \\ & = \sum_{j \in S_g^{sc}} \left( \sum_{i \in S_g^m} \alpha_{ji} \beta_i \right) |ET_{SC} j\rangle \end{aligned}$$

From equation (13) it is evident that to have a bound state at the interface the vector  $\beta$  must belong to the null space of the reduced matrix  $\alpha_r$ , which is the  $S_g^{sc} \times S_g^m$  upper left part of the original matrix  $\alpha$  since the matrices  $PET_M$  and  $ET_{SC}$  are organized to have the eigenstates with the largest eigenvalues as column vectors to the left. In the case that the two subspaces  $S_g^{sc}$  and  $S_g^m$  have the same dimension a bound state at the interface is characterized by the vanishing of the determinant of  $\alpha_r$

$$\text{Bound states:} \quad \det(\alpha_r) = 0. \quad (14)$$

Plots of the wavefunctions with values of  $(q, \epsilon)$  that satisfy Eqn. (14) verifies that these states indeed are bound to the interface (not shown). The following explicit values of the input parameters are chosen:  $t = 1$ ,  $\Delta_d = 0.14$ ,  $M = 2.0$  and  $\mu = -0.99$  (for simplicity we ignore next-nearest neighbor coupling). Figure 1a shows the determinant plotted as a function of energy for the  $\{100\}$  interface. There are bound states close to the superconducting gap edge that disperses downward in a cosine form (Figure 1b). These are the well-known de Gennes/Saint-James states existing on the surface of an insulator and a superconductor<sup>13,14</sup>.

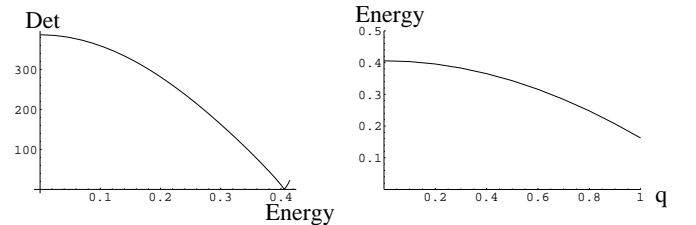


FIG. 1.  $\{100\}$  interface between an antiferromagnet and a d-wave superconductor: a) Determinant of  $\alpha_r$  as a function of energy  $\epsilon$  for  $q = 0.1$ . There is a de Gennes/Saint-James bound state close to the superconducting gap edge. As seen in b), their dispersion has the expected downward cosine form until it merges with the continuum.

The induction of additional gap symmetries, extended s-wave or p-wave, near the  $\{100\}$  interface of a d-wave superconductor and an antiferromagnet has been studied self-consistently by Kuboki<sup>15</sup>. These local gap perturbations will slightly modify the graphs in Figure 1. There

is no spin splitting of the dGSJ mode in this geometry. We turn now to the more interesting configuration of a  $\{110\}$  interface. Allowing for a possible interface induced sub-gap order with extended s-wave symmetry the Bogoliubov-de Gennes equations have the form

$$\epsilon_\sigma u_{q\sigma}(x) = -2t \cos(p) (u_{q\sigma}(x+1) + u_{q\sigma}(x-1)) - \mu u_{q\sigma}(x) + \sigma M_x u_{q\sigma}(x) \quad (15)$$

$$\begin{aligned} & - 2i \sin(q) (\Delta_{x+1,x}^d v_{q\sigma}(x+1) - \Delta_x^d v_{q\sigma}(x-1)) + 2i \cos(q) (\Delta_{x+1,x}^s v_{q\sigma}(x+1) + \Delta_x^s v_{q\sigma}(x-1)) \\ \epsilon_\sigma v_{q\sigma}(x) = & 2t \cos(p) (v_{q\sigma}(x+1) + v_{q\sigma}(x-1)) + \mu v_{q\sigma}(x) + \sigma M_x v_{q\sigma}(x) \quad (16) \\ & - 2i \sin(q) (\Delta_{x+1,x}^{*d} u_{q\sigma}(x+1) - \Delta_x^{*d} u_{q\sigma}(x-1)) - 2i \cos(q) (\Delta_{x+1,x}^{*s} u_{q\sigma}(x+1) + \Delta_x^{*s} u_{q\sigma}(x-1)) \end{aligned}$$

These equations are diagonal in the Fourier component  $q$  obtained after Fourier transforming parallel to the  $\{110\}$  interface since there is no staggering of the moments along a diagonal line in a square antiferromagnetic lattice. In Figure 2 we plot again the determinant of the reduced matrix  $\alpha_r$  as a function of energy  $\epsilon$  when  $\Delta^s = 0$ . As seen the spin degeneracy of the ZEBS (dashed curve) is lifted at a  $\{110\}$  AF/dSC interface. As opposed to the usual dGSJ states in Figure 1, this splitting is also caused by the fact that a  $\{110\}$  interface belongs to only one sublattice whereas the  $\{100\}$  interface studied above contains the same amount of spin up and down sites.

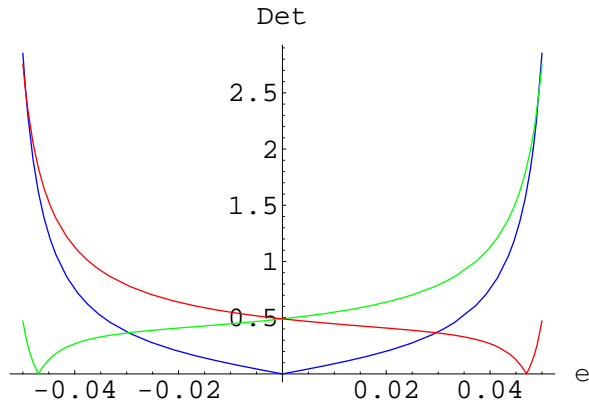


FIG. 2. Determinant of  $\alpha_r$  versus the energy  $\epsilon$  for the  $\{110\}$  AF/dSC interface. Again this is plotted inside the superconducting gap and with  $q = 0.1$ . The dashed curve is the usual case of an I/dSC interface which clearly contains a ZEBS (the insulator state is obtained by performing the substitution  $M_n \rightarrow -M_n$  for the hole part of the BdG equations only). The solid curves show the spin splitting of the ZEBS for this particular value of  $q$ .

The splitting of the ZEBS by  $\Delta^s$ -mixing in the usual situation of a I/dSC interface has been extensively studied in the literature<sup>7-9</sup>. It is also well-known that a magnetic field further splits the ZEBS<sup>5</sup>. The above spin splitting at AF/dSC interfaces is similar to this magnetic field effect in the sense that the magnetic interface effectively

acts as a local magnetic field. A similar effect caused by a correlation induced magnetization near the interface in the case of a I/dSC surface was discussed by Honerkamp *et.al*<sup>9</sup>. This “Zeeman” effect is also directly related to the split zero energy Andreev mode observed in the center of vortex cores of underdoped cuprates where local antiferromagnetism has been shown to exist<sup>17-22</sup>. To the best of our knowledge there has been no self-consistent calculation investigating any  $\{110\}$  AF/dSC interface induced subdominant order parameters.

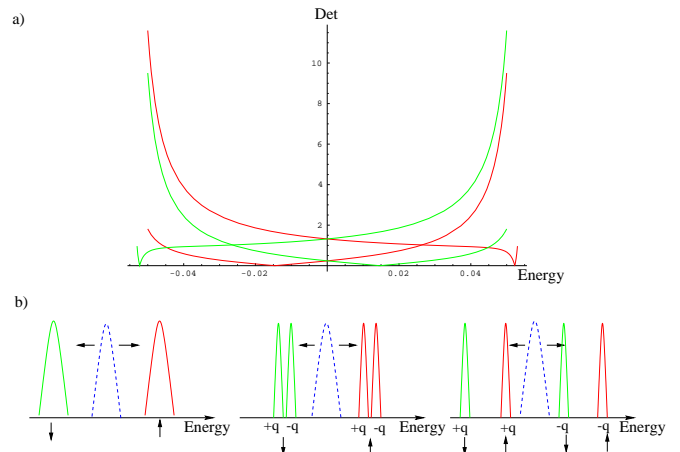


FIG. 3. a) Same as in Figure 2, but with an induced extended s-wave gap function near the interface, i.e.  $d \rightarrow d + is$ . For clarity we do not show the original ZEBS (dashed curve from Fig. 2). b) Schematic representation of the splitting of the original zero energy Andreev bound state (dashed curve): 1) The antiferromagnetic interface breaks the spin degeneracy, as shown in Fig. 2. 2) Induction of a possible sub-dominant s-wave gap parameter  $\Delta^s$  further splits the spin up/down states by breaking the directional degeneracy. 3) Only when  $\Delta^s$  exceeds a critical value is an interface current induced. In this last figure, which corresponds to the situation from a),  $\Delta^s$  is equal to  $\Delta^d$  on the interface and decreases linearly to zero within 20 sites of the interface.

However, we know from the study of I/dSC surfaces<sup>7,16</sup> that the strong pair breaking effects of a  $\{110\}$  geometry,

as opposed to a  $\{100\}$  surface, tends to stabilize the subdominant s-wave component. Thus, even though there is no Fermi surface instability begging for removal of the ZEBS from the Fermi level in the case of a AF/dSC  $\{110\}$  interface, one should still consider the effect of an additional local superconducting order parameter *is* competing with the splitting caused by the magnetism. The consequences of this competition for the ZEBS are discussed in Figure 3.

The induction of a surface current is a well-known consequence of the time reversal symmetry broken state of I/dSC interfaces<sup>7,8</sup>. However, for the AF/dSC interface with a locally induced  $d \pm is$  order parameter there is a critical value of  $\Delta_c^s$  before a current runs along the interface<sup>23</sup>. In Figure 3a we show the situation when the induced  $\Delta^s$  has exceeded this critical value. Figure 3b is a schematic representation of the splitting of the original ZEBS with the first sketch corresponding to the parameters from Fig. 2 and the last sketch to those from Fig 3a. We stress that only a self-consistent model calculation can determine the magnitude of the directional splitting caused by *is* compared to the spin splitting caused by the antiferromagnetism, and hence the relevancy of the interface current.

In conclusion we have set up a simple method so determine the existence of bound states at the interfaces of d-wave superconductors and antiferromagnets. In particular we studied the energetics of the notorious zero energy mode bound to  $\{110\}$  I/dSC interfaces first discovered by Hu<sup>4</sup>. This state is always spin split when the insulator is an antiferromagnet and is analogous to the split states found around the magnetic vortex cores of YBCO and BSCCO crystals. In the case of an array of junctions corresponding to a periodic domain of vertical or diagonal stripes these states will hybridize and eventually form a band. A current along the interface exists only when the effect of a competing, interface induced *is* component exceeds the spin splitting.

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<sup>1</sup> Z-X. Shen, D.S. Dessau, B.O. Wells, D.M. King, W.E. Spicer, A.J. Arko, D. Marshall, L.W. Lombardo, A. Kapitulnik, P. Dickinson, S. Doniach, J. diCarlo, A.G. Loeser, and C.H. Park, Phys. Rev. Lett. **70**, 1553 (1993).

<sup>2</sup> D.J. van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).

<sup>3</sup> S. Kashiwaya, Y. Takana, M. Koyanagi, and M. Kajimura,

Phys. Rev. B **53**, 2667 (1996).

<sup>4</sup> C-R.Hu, Phys. Rev. Lett. **72**, 1526 (1994).

<sup>5</sup> M. Covington, M. Aprili, E. Paraonu, L.H. Greene, F. Xu, J. Zhu, and C.A. Mirkin, Phys. Rev. Lett. **79**, 277 (1997).

<sup>6</sup> For a review see, T. Löfwander, V.S. Shumeiko, and G. Wendin, Supercond. Sci. Technol. **14**, R53 (2001).

<sup>7</sup> M. Fogelström, D. Rainer and J.A. Sauls, Phys. Rev. Lett. **79**, 281 (1997); M. Fogelström and S-K. Yip, Phys. Rev. B. **57**, R14060 (1998).

<sup>8</sup> M. Sigrist, Prog. Theo. Phys. **99**, 899 (1998).

<sup>9</sup> C. Honerkamp, K. Wakabayashi, and M. Sigrist, Europhys. Lett. **50** (3), 368 (2000).

<sup>10</sup> B. Lake, H.M. Rønnow, N.B. Christensen, G. Aeppli, K. Lefmann, D.F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, and T.E. Mason, Nature **415**, 299 (2002).

<sup>11</sup> B. Khaykovich, Y.S. Lee, R. Erwin, S-H. Lee, S. Waki-moto, K.J. Thomas, M.A. Kastner, and R.J. Birgeneau, cond-mat/0112505.

<sup>12</sup> E. Merzbacher, "Quantum Mechanics", Wiley Int. Edition, (1970).

<sup>13</sup> P.G. de Gennes and D. Saint-James, Phys. Lett. **4**, 151 (1963).

<sup>14</sup> The dGSJ states are usually thought of as existing in a narrow normal region (within the superconducting coherence length  $\xi$ ) from the surface. However, it is known that these states survive in the limit  $\xi \rightarrow 0$ . See also<sup>6</sup>.

<sup>15</sup> K. Kuboki, J. Phys. Soc. Jap. **68**, 3150 (1999).

<sup>16</sup> M. Matsumoto and H. Shiba, J. Phys. Soc. Jap. **64**, 3385 (1995), **64**, 4867 (1995), **65**, 2194 (1996).

<sup>17</sup> S.H. Pan, E.W. Hudson, A.K. Gupta, K-W. Ng, H. Eisaki, S. Uchida, and J.C. Davis, Phys. Rev. Lett. **85**, 1536 (2000).

<sup>18</sup> I. Maggio-Aprile, C. Renner, A. Erb, E. Walker, and Ø. Fischer, Phys. Rev. Lett. **75**, 2754 (1995).

<sup>19</sup> B.M. Andersen, H. Bruus, and P. Hedegård, Phys. Rev. B **61**, 6298 (2000).

<sup>20</sup> J-X. Zhu and C.S. Ting, Phys. Rev. Lett. **87**, 147002 (2001).

<sup>21</sup> R.I. Miller, R.F. Kiefl, J.H. Brewer, J.E. Sonier, J. Chakhalian, S. Dunsiger, G.D. Morris, A.N. Price, D.A. Bonn, W.H. Hardy, and R. Liang, Phys. Rev. Lett. **88**, 137002 (2002).

<sup>22</sup> V.F. Mitrovic, E.E. Sigmund, M. Eschrig, H.N. Bachman, W.P. Halperin, A.P. Reyes, P. Kuhns, and W.G. Moulton, Nature **413**, 501 (2001).

<sup>23</sup> Here we assume the large effect is the spin splitting since  $M$  gives rise to the Hubbard gap in the bulk antiferromagnet, and  $\Delta^s$  is an extra perturbation. In the opposite case it would take a critical magnetization  $M_c$  to prevent the interface current induced by  $\Delta^s$ .